

2,2,4-Trimethyl-1,3-pentanediol
144-19-4 | DTXSID8027113

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.80e-03 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.07e-01

Confidence level: 4.67e-01

Nearest Neighbors from the Training Set

Image not found

Heptane

Measured: 4.50e-03

Predicted: 42.3

Image not found

Dicofol

Measured: 1.00e-04

Predicted: 2.79e-07

Image not found

2,4,4-Trimethyl-1-pentene

Measured: 1.30e-02

Predicted: 45.3

Image not found

MCPB

Measured: 3.00e-03

Predicted: 1.30e-06

Image not found

Toluene

Measured: 8.06

Predicted: 22.2